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REGULARIZED FINITE ELEMENT METHOD FOR SINGULAR PERTURBED CONVECTION-DIFFUSION-REACTION MODELS WITH NONUNIFORM SOURCES

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In this paper we present finite element scheme which combines Tikhonov regularization with method of characteristics to reduce Peclet number of original problem to needed value. This will disable oscillations of approximate solution and thus make possible of application standard finite element method with relatively low element count to singular perturbed problems.

Key words: finite element method, Galerkin method, P?clet criteria, well posed problem, diffusion-advection-reaction boundary value problem, stabilization schemes, Tikhonov regularization, method of characteristics, transport equation.

1. Introduction

Convection-diffusion-reaction boundary value problems with large Peclet number (i.e. with convection dominated over diffusion) appear in many applications. Large Peclet number causes existence of boundary layers in the problem domain, when solution experience large gradients. This complicated structure of the solution is the root cause of oscillations which are present in finite element approximation on coarse meshes. To make it possible, to match this solution structure with uniform meshes we will need very large elements count, making thus the process of finding solution very computationally-heavy.

There are many ways to deal with boundary layers. One of the most universal and powerful is to use adaptive meshes. In this case we adapt in some manner finite element mesh (or even approximation degree) to cover boundary layers with more nodes. This process will reflect more precisely solution behavior in boundary layer on one hand and it will not add additional nodes in the part of domain, when solution is sufficiently smooth on the other hand. Such approach can give us huge increase of computational efficiency by operating with enough smaller counts of finite elements. The other family of approaches is stabilization methods like streamline diffusion method [1]. In this case we modify in some way the variational equation, to incorporate there some penalty terms which specially forces approximate solution to be more smooth. This stabilization can be done on coarse meshes and lead to quite adequate approximations. Stabilization methods often lead us to add some artificial diffusion to the original equation. We may also mention here discontinuous Galerkin fininte element methods, which also uses penalty terms in their variational formulation, which is natural in this case, as they are used to make some weak connectivity between the elements [2, 6].

Here we present a new approach, which is somehow similar to stabilization schemes, but instead it uses more a posteriori information about the solution to construct mentioned penalty terms. One difference to mention is that implemented method is not consistent, unlike well-known stabilization schemes, or discontinuous finite element methods, i.e. the exact solution of original problem does not satisfy exactly variational formulation, which we use for approximation.

2. Problem setting

Let $\Omega \in \mathbb{R}^2$ be an open bounded convex simply connected domain. We consider the following boundary value problem:

$$\begin{cases} \text{Find function } \; u : \mathbb{R}^2 \to \mathbb{R} \; \text{ such that:} \\ -\mu\Delta u + \vec{\beta}(x)\cdot\nabla u + \sigma u = f(x) \quad \text{on} \quad x \in \Omega \\ u|_{\partial\Omega} = 0. \end{cases} \tag{1}$$

Positive numbers $\mu, \sigma \in \mathbb{R}$ are coefficients of diffusion and reaction respectively. Scalar and vector-valued functions f and $\vec{\beta}$ are representing source term and convection speed correspondingly. We may consider μ as a small parameter of a given problem [3]. Additionally, we suppose, that vector field $\vec{\beta}$ has zero divergence, i.e. $\nabla\cdot\vec{\beta} = 0$ on Ω. From the physical point of view, it means, that considered convection flow is non-compressible.

In this paper we do not concentrate our attention on the function classes and other conditions which we need to meet to make the problem (1) well posed, as this was discussed in many other articles [2, 4, 11]. We suppose, that problem data is such, that (1) has unique weak solution.

3. Weak formulation

Let us define space $V := H_0^1(\Omega)$ with standard Sobolev norm $\|\bullet\|_V$. By multiplying the equation from (1) by arbitrary $v \in V$ and using first Greens's identity to the first term, we derive the following variational formulation

$$\begin{cases} \text{Find } \; u \in V \; \text{ such that} \\ a(u,v) = \langle l, v\rangle \quad \forall v \in V, \end{cases} \tag{2}$$

where

$$\begin{cases} a(u,v) = \displaystyle\int_\Omega (\mu\nabla u\cdot\nabla v + \vec{\beta}v\cdot\nabla u + \sigma uv)dx \\ \langle l, v\rangle = \displaystyle\int_\Omega fvdx. \end{cases} \tag{3}$$

It is not hard to show, that if $\vec{\beta}(x)$ is bounded, then bilinear form $a : V^2 \to \mathbb{R}$ is bounded. It is also simply to show that $a(u,v)$ is V-elliptical and linear functional l is bounded. Next, by applying Lax-Milgram theorem, we conclude that the problem (2) is well-posed. In the next theorem we prove that, $a(u,v)$ is V-elliptical, providing needed lower bound for the energy norm.

Proposition 1. *Suppose, that μ is a small parameter, $\mu < \sigma$. Then $a(u,v)$ is V-elliptical and $a(u,u) \geq \mu\,\|u\|_V^2$.*

Proof. Let us apply Gauss-Ostrogradsky theorem to the function $u^2\vec{\beta}$. We will have:

$$\int_\Omega (2u\nabla u\cdot\vec{\beta} + u^2\nabla\cdot\vec{\beta})\,dx = \int_{\partial\Omega} u^2\vec{\beta}\cdot\vec{n}\,d\gamma, \tag{4}$$

where $\vec{n} : \partial\Omega \to \mathbb{R}^2$ is a unit vector of outward normal to the boundary of domain Ω. Since $\nabla \cdot \vec{\beta} = 0$ on Ω and $u|_{\partial\Omega} = 0$ for $u \in V$ we obtain, that

$$\int_\Omega u\nabla u \cdot \vec{\beta}\, dx = 0, \quad \forall u \in V \tag{5}$$

and as an immediate conclusion we finish the proof

$$a(u, u) = \int_\Omega (\mu|\nabla u|^2 + \sigma u^2)dx \geq \min\{\mu, \sigma\} \|u\|_V^2 = \mu \|u\|_V^2 . \tag{6}$$

□

It is important to note, that in the case, when bilinear form is symmetric using known facts from variational calculus we can reformulate the weak problem (2) as an equivalent minimization problem

$$\begin{cases} \text{Find } \ u \in V \ \text{ such that} \\ F(u) \leq F(v) \quad \forall v \in V \end{cases} \tag{7}$$

where $F(u) := a(u, u) - 2\langle l, u\rangle$.

4. Tikhonov regularization

Classical Tikhonov regularization is used to obtain approximate solution of the equation $Au = f$, where operator A^{-1} is not bounded, or has large condition number. In such cases any small perturbation of f can lead to very large difference in obtained solution with respect to original one and specially to large values of $\|u\|$. Tikhonov proposed to modify standard least squares method (i.e. minimization of $\|Au - f\|^2$) with additional terms, which will act as penalty with respect of the value of $\|u\|$. Such approach will reduce the sensitivity of obtained solution to the errors in problem data f. To be more precise, the basic Tikhonov regularization problem [8] is formulated as follows

$$\begin{cases} \text{Find } \ u \ \text{ such that} \\ \|Au - f\|^2 + \lambda\|u\|^2 \to \min . \end{cases} \tag{8}$$

Here and next $0 < \lambda \in \mathbb{R}$. It can be, that we already have some a priori knowledge about solution. For example, we know, that true solution is close to some other value u_0. In such case we can use Tikhonov-type regularization with modified penalizing term [7, 9] instead of (8)

$$\begin{cases} \text{Find } \ u \ \text{ such that} \\ \|Au - f\|^2 + \lambda\|u - u_0\|^2 \to \min . \end{cases} \tag{9}$$

We propose to use generalized regularization procedure (9) with respect of problem (7) and standard Sobolev norm, i.e. we consider the following problem

$$\begin{cases} \text{Find } \ u^* \in V \ \text{ such that} \\ J(u^*) := a(u^*, u^*) - 2\langle l, u^*\rangle + \lambda \|u^* - u_0\|_V^2 \to \min \end{cases} \tag{10}$$

The function u_0 is not necessary to be from space V. Let us define domain part $\Gamma_0 := \{x \in \partial\Omega | \vec{n}(x) \cdot \vec{\beta}(x) < 0\}$, i.e. Γ_0 is the part of boundary, where the vector $\vec{\beta}$ is oriented to the internal part of $\partial\Omega$. We suppose, that the set Γ_0 is connected. We also suppose, that for each point $x \in \Omega \cup (\partial\Omega \setminus \Gamma_0)$ integral curve of vector field $\vec{\beta}$, which passes through x, starts in some point $y \in \Gamma_0$. The last condition will eliminate existence of closed integral curves of $\vec{\beta}$ in Ω. Assuming sufficient smoothness of problem data, we propose here the special choose of u_0 as a solution of the following boundary problem

$$\begin{cases} \text{Find function } \ u_0 \in C^1(\Omega) \ \text{ such that:} \\ \vec{\beta}(x) \cdot \nabla u_0 + \sigma u_0 = f(x) \quad \text{on} \ \ x \in \Omega \\ \ u_0|_{\Gamma_0} = 0, \end{cases} \tag{11}$$

which actually can be considered as a restriction of some Cauchy problem (we restrict Cauchy initial data from some curve on whole plane to just its part Γ_0 and we are trying to find solution not on whole plane but just in Ω, which, in fact, contains curve Γ_0).

We will call (11) *reduced problem* (which is actually transport equation [10]).

5. Properties of regularized problem

Let us consider formulation of problem (10) in the form of variational equation. We denote by $(u,v)_V := \int\limits_{\Omega} (uv + \nabla u \cdot \nabla v)\, dx$ standard Sobolev scalar product. By equating first variation of functional J to zero, we transform (10) to the following form

$$\begin{cases} \text{Find} \ \ u^* \in V \ \text{ such that} \\ a(u^*, v) + \lambda(u^*, v)_V = \langle l, v\rangle + \lambda(u_0, v)_V \quad \forall v \in V. \end{cases} \tag{12}$$

We also can use such problem in general case, i.e. when bilinear form is not symmetric. It is not hard to see, that bilinear form $b(u,v) := a(u,v) + \lambda(u,v)_V$ is bounded on V and V-elliptic. Functional $\langle p, v\rangle := \langle l, v\rangle + \lambda(u_0, v)_V$ is also bounded and linear. Thus, applying Lax-Milgram theorem shows that problem (12) is well-posed. For the V-ellipticity we have:

$$b(v,v) \geq \ (\lambda + \mu)\, \|v\|_V^2 \tag{13}$$

Let us subtract equation (2) from (12). We will get

$$a(u^* - u, v) + \lambda(u^*, v)_V = \lambda(u_0, v)_V \tag{14}$$

Next, we subtract the term $\lambda(u,v)_V$ from both sides of (14)

$$b(u^* - u, v) = a(u^* - u, v) + \lambda(u^* - u, v)_V = \lambda(u_0 - u, v)_V \tag{15}$$

Taking $v := u^* - u \in V$ and using (13) on the left side together with Cauchy-Schwarz inequality on the right side we obtain

$$(\lambda{+}\mu)\, \|u^* - u\|_V^2 \leq b(u^*{-}u, u^*{-}u) = \lambda(u_0 - u, u^* - u)_V \leq \lambda \|u_0 - u\|_V \|u^* - u\|_V \tag{16}$$

or, after simplification

$$\|u^* - u\|_V \leq \ \frac{\lambda}{\lambda + \mu} \|u_0 - u\|_V. \tag{17}$$

Since $\lambda/(\lambda + \mu) < 1$, we get:

$$\|u^* - u\|_V \ \ < \ \ \|u_0 - u\|_V \tag{18}$$

The last equality is clearly natural, since it is logically to suppose, that accuracy of regularization procedure will be dependent on the accuracy of u_0.

Note, that taking into account (17) we can build the sequence of functions $\{u_i\}$, defined as a solutions of the set of the following recurrent variational problems

$$\begin{cases} \text{Find} \;\; u_i \in V \;\; \text{such that} \\ a(u_i, v) + \lambda(u_i, v)_V = \langle l, v\rangle + \lambda(u_{i-1}, v)_V \quad \forall v \in V. \end{cases} \tag{19}$$

For those functions, the following inequality holds

$$\|u_i - u\|_V \leq \frac{\lambda}{\lambda + \mu}\|u_{i-1} - u\|_V \tag{20}$$

and furthermore:

$$\|u_i - u\|_V \leq \left(\frac{\lambda}{\lambda + \mu}\right)^i \|u_0 - u\|_V. \tag{21}$$

So, we have, that $\|u_i - u\|_V \to 0$ as $i \to \infty$. We should note, than convergence is slow in this case. Furthermore, we will show in the next chapters, that this iterative procedure is not practical except of the first step, i.e. the problem (12), which can be used successfully in practical computations.

One interesting question is, how the $\|u_0 - u\|_V$ depends on μ. Investigating this is out of scope of this article. We should note, that for L_2 norm in 1D case we can simply show using asymptotic expansions, that $\|u_0 - u\|_0 = O(\mu)$ as $\mu \to 0$. The last fact is natural, as we expect, that the solution of the reduced problem should match the solution of original one more precisely as diffusive part is decreasing. Investigating similar fact for Sobolev norm is not so obvious, because of presence of derivative terms in the norm, which can be large inversely proportional to the thickness of boundary layer. In general, it can be, that even $\|u_0 - u\|_V \to \infty$ as $\mu \to 0$. To show that, let us just consider the 1D equation $-\mu u'' + u' = 1$ on $(0, 1)$ with boundary conditions $u(0) = u(1) = 0$. It is easy to find solution $u(x) = x - (e^{x/\mu} - 1)/(e^{1/\mu} - 1)$. Corresponding solution of reduced problem is $u_0(x) = x$. For such case we can transparently verify that $\|u_0 - u\|_V \to \infty$ as $\mu \to 0$.

Making estimates in the form of (17) but with weaker norm (i.e. without derivatives) will be an open question for now. Let us look to the characterization of singular perturbations in the given problem. Peclet number is the main measure in our case for that. It is defined as a ratio of convection speed to diffusion speed. For the original and regularized problems Peclet numbers are the following

$$Pe_{orig} = \frac{\left\|\vec{\beta}\right\|_\infty diam\ \Omega}{\mu} \quad \text{and} \quad Pe_{reg} = \frac{\left\|\vec{\beta}\right\|_\infty diam\ \Omega}{\mu + \lambda}. \tag{22}$$

We can clearly see, that while Pe_{orig} can be very large, when μ is small, we always can tune up Pe_{reg} to be arbitrary needed number in the interval $(0, Pe_{orig}]$ by choosing appropriate λ. Using this fact we can see, that we can force regularized problem to not be singular perturbed, making the application of classical finite element approximations on the coarse uniform meshes possible.

6. Approximate solution of reduced problem

Consider the case when vector field $\vec{\beta} \neq 0$ in any point on Ω. Let us construct some parametrization of 1D set Γ_0. Let's define function $[0, mes\Gamma_0] \ni \eta \mapsto \rho(\eta) = (\rho_1(\eta), \rho_2(\eta)) \in \bar{\Gamma}_0$ which maps parameter η bijectively onto the $\bar{\Gamma}_0$. Also the direction of increasing parameter η corresponds to moving along the Γ_0 in the counterclockwise direction with respect to whole domain boundary $\partial\Omega$. For each value of η we can construct integral curve of vector field $\vec{\beta}$: $x(t,\eta) = (x_1(t,\eta), x_2(t,\eta)) \in \Omega$ as a solution of the following Cauchy problem

$$\begin{cases} \dfrac{\partial x(t,\eta)}{\partial t} = \vec{\beta}(x(t,\eta)), \\ x(0,\eta) = \rho(\eta). \end{cases} \tag{23}$$

Let us consider now reduced problem which we introduced before and define the function $z(t,\eta) = u_0(x(t,\eta))$. Taking into account (23) and using chain rule, we can derive the following:

$$\frac{\partial z(t,\eta)}{\partial t} = \vec{\beta}(x(t,\eta)) \cdot \nabla_x u_0(x(t,\eta)) \tag{24}$$

Using the last equality and (23), we can rewrite reduced problem (11) as an Cauchy problem for system of three scalar ODEs

$$\begin{cases} \dfrac{\partial x(t,\eta)}{\partial t} = \vec{\beta}(x(t,\eta)), \\ \dfrac{\partial z(t,\eta)}{\partial t} = f(x(t,\eta)) - \sigma z(t,\eta), \\ x(0,\eta) = \rho(\eta), \\ z(0,\eta) = 0. \end{cases} \tag{25}$$

The method of reducing the first-order PDE to the system of ODEs which we used is called in the literature as *method of characteristics* [5]. Curves $x(t,\eta)$ are called the characteristic curves of original PDE.

From the classical theory of differential equations we know, that for sufficiently smooth data, problem (11) has unique solution. In that case it is obvious, that the solution surface is an union of the solution curves of problem (25).

We will use introduced method of characteristics to solve (11). The steps are the following:

1. generate some 1D mesh of points on the curve Γ_0;
2. for each of generated point build approximate solution of (25), using some methods like Runge-Kutta or similar;
3. interpolate solutions to obtain single approximation (for example, we can use splines for that).

7. Finite element approximation of regularized problem

For the experiment, we used Galerkin method [2,6] for discretization of problem (12). For local approximation we used triangular finite elements with linear basis functions [2]. Regularization parameter λ was selected experimentally and the automatic selection was not considered.

Let us consider now the iteration procedure which was introduced above. We can clearly see, that exactly the same inequality as (17) will be true for Galerkin approximations and the convergence result will be the same, i.e. approximate solutions of regularized problems will converge to the Galerkin solution of original singular perturbed problem. Thus, as the original approximation has high oscillations, it is not practical to use such iteration procedure.

8. Numerical examples

It is naturally, that constructed method can be specially used for the singularly perturbed problems, where the solution of reduced equation has complex, but still regular structure. Otherwise, when the solution of reduced equation is almost constant, we can just use $u_0 = 0$ for regularization, i.e. use ordinary Tikhonov regularization. For interested case, we can just use highly non-uniform source term f to show the specific of the method and it's applications.

We implemented proposed algorithm for both 1D and 2D. We used Python programming language with Scipy library to perform all auxiliary tasks and famous J.R.Shewchuk's library for building Delaunay triangulations. 1D case is much simpler, but it is very good for the situation, when we need the possibility to make precise visual exploration of obtained approximations.

(1D example): We used the following data:

$\Omega = (0,1), \quad \mu = 1, \quad \vec{\beta} = 10^3, \quad \sigma = 10^2, \quad f = 10^5 cos(2.25\pi x), \quad \lambda = 30.$

Approximation was found on uniform mesh with 20 elements. In the Fig.1 we show regularized and original approximations on 20 elements and for the reference also approximation on highly refined mesh – on 200 elements and the approximate solution of reduced problem. In addition, we show the regularized approximation for the case $u_0 := 0$. We can clearly see, that using a posteriori information from the solution of reduced problem can be critical, to obtain accurate approximation.

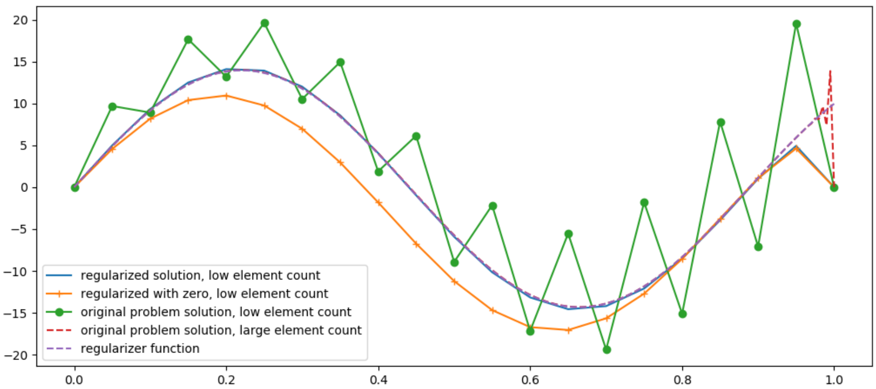

Fig. 1. 2D example. We used the following data: $\Omega = (0,1)^2, \quad \mu = 1, \quad \vec{\beta} = (10^3, 10^3),$ $\sigma = 10^2, \quad f = 10^5 \cos(2.25\pi x)\cos(2.25\pi y), \quad \lambda = 30$

Coarse mesh was built using 150 triangles with areas not larger than 0.01 and highly refined mesh for more accurate solution was built with 5193 triangles with areas not larger than 0.0003. Results are present in Figures 2, 3 and 4.

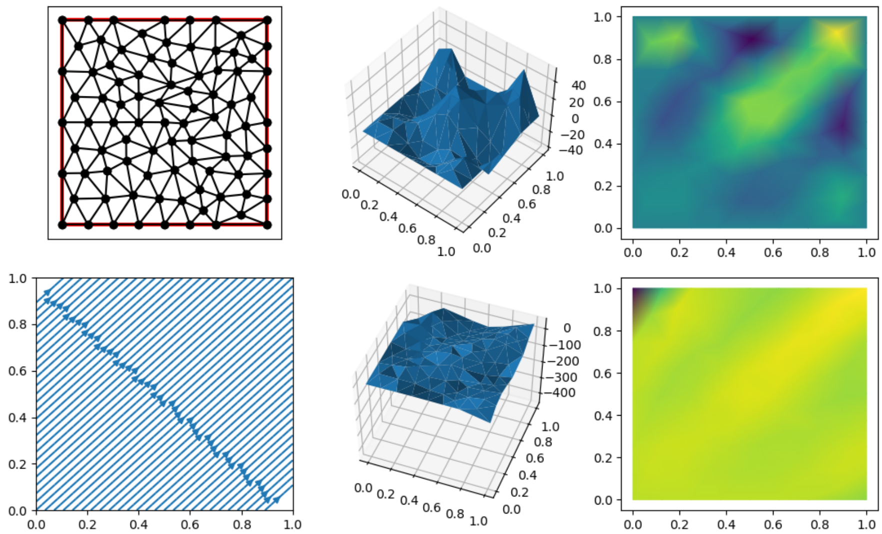

Fig. 2. Regularized approximate solution on coarse mesh. On the first row we show mesh, which was used, solution graph in 3D and corresponding heatmap, which shows by color obtained substance density. On the second row we visualize vector field $\vec{\beta}$, graph of obtained interpolated approximation to the u_0 in 3D and corresponding heatmap

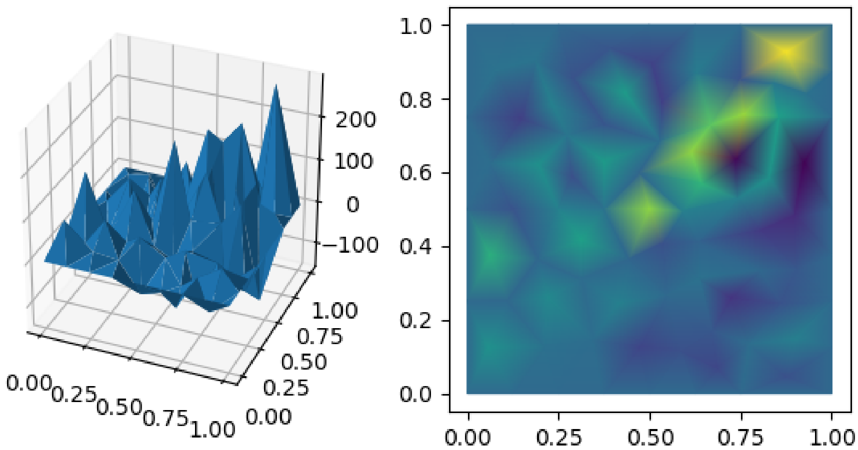

Fig. 3. Non-regularized approximate solution on coarse mesh. We clearly see highly oscillated approximation, which is completely not usable

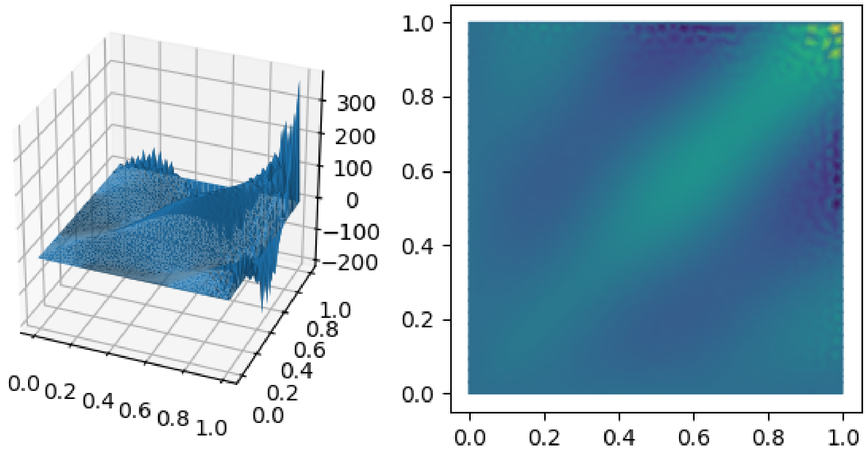

Fig. 4. Non-regularized approximate solution on highly refined mesh. We still see oscillations near the boundary layer, due to which the scaling in the heatmap reduced the colors intensity for most points

9. Conclusions

In this paper we constructed new approach for solving singular perturbed diffusion-convection-reaction problems. We present finite element scheme which combines Tikhonov regularization with method of characteristics to reduce Peclet number of original problem to needed value. This will disable oscillations of approximate solution and thus make possible of application standard finite element method with relatively low element count to singular perturbed problems. We provided some initial error estimates and verified the method on several numerical experiments.

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РЕГУЛЯРИЗОВАНИЙ МЕТОД СКІНЧЕННИХ ЕЛЕМЕНТІВ ДЛЯ СИНГУЛЯРНО ЗБУРЕНИХ МОДЕЛЕЙ КОНВЕКЦІЇ-ДИФУЗІЇ-РЕАКЦІЇ З НЕРІВНОМІРНИМ РОЗПОДІЛОМ ДЖЕРЕЛ ДОМІШКИ

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Побудовано схему методу скінченних елементів, яка поєднує регуляризацію Тихонова з методом характеристик для зменшення числа Пекле вихідної задачі до необхідного значення. Такий підхід дає змогу погасити осциляції наближеного розв'язку, і, отже, робить можливим застосування стандартного методу скінченних елементів із порівняно малою кількістю елементів до сингулярно збурених задач.

Ключові слова: метод скінченних елементів, метод Гальоркіна, критерій Пекле, коректно сформульована задача, модель конвекції-дифузії-реакції, схеми стабілізації, регуляризація Тихонова, метод характеристик, рівняння переносу.